On the efficient computation of the projector over the Birkhoff polytope

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Optimization over Birkhoff polytope

Consider optimization problem:

$$\min\{f(X) \mid X \in \mathfrak{B}_n\}$$

Birkhoff polytope:

$$\mathfrak{B}_n := \{X \in \Re^{n\times n} \mid Xe = e,\ X^T e = e, X \geq 0\}$$

$e \in \Re^n$: the vector of all ones

$f : \Re^{n\times n} \to (-\infty, +\infty]$, possibly nonconvex, nonsmooth

Permutation matrices:

$$\mathfrak{D}_n := \{X \in \Re^{n\times n} \mid Xe = e,\ X^T e = e, X_{ij} \in \{0, 1\}\}$$

Convex hull: [Birkhoff, 1946 & J. von Neumann, 1953]

$$\mathfrak{B}_n = \mathrm{conv}(\mathfrak{D}_\mathrm{n})$$

Examples

(i) Graph based Clustering, given affinity matrix K
[Zass et al., NIPS, 2006]:

$$\min\left\{\|X-K\|_F^2 \mid X \in \mathfrak{B}_n\right\}$$

[Wang et al., KDD, 2016]: given $k \geq 0$,

$$\min\left\{\|X-K\|_F^2 + \gamma\|I-X\|_* + r\|X\|_F^2 \mid X \in \mathfrak{B}_n,\ \mathrm{Tr}(X)=k\right\}$$

(ii) Graph Matching, adjacency matrices A, B, [Fiori et al., NIPS, 2013]:

$$\min\left\{\|AX-XB\|_F^2 \mid X \in \mathfrak{B}_n\right\}$$

$$\min\left\{\sum_{i,j}\|((AX)_{ij},(XB)_{ij})\|_2 \mid X \in \mathfrak{B}_n\right\}$$

Examples

(iii) Relaxation of the seriation problem, 2-SUM minimization, given symmetric, binary matrix A, [Fogel et al., NIPS, 2013], [Lim & Wright, 2014]:

$$\min\{\langle Xg,\, L_A Xg\rangle \mid X \in \mathfrak{B}_n\}$$

$g = (1, \ldots, n)^T$ and $L_A = \mathrm{diag}(Ae) - A$

Relaxations of the quadratic assignment problems (QAP)...

Difficulties: constrained minimization, n^2 unknown variables in X, large-scale even when $n = 10^3$

Projection onto $\mathfrak{B}_n$

Metric projector over $\mathfrak{B}_n$: given $G \in \Re^{n\times n}$

$$\Pi_{\mathfrak{B}_n}(G) := \arg\min \left\{ \frac{1}{2}\|X - G\|_F^2 \mid X \in \mathfrak{B}_n \right\}$$

Easy computation of $\Pi_{\mathfrak{B}_n}(G)$ "$\Longrightarrow$" first order methods for

$$\min\{f(X) + \delta_{\mathfrak{B}_n}(X)\}$$

$\delta_{\mathfrak{B}_n}(\cdot)$: indicator function over $\mathfrak{B}_n$

PG, APG (FISTA), ADMM, splitting methods ...

Generalized Jacobian $\partial\Pi_{\mathfrak{B}_n}(G)$ "$\Longrightarrow$" second order methods

(sparse) semismooth (generalized) Newton methods

Computation of $\Pi_{\mathfrak{B}_n}(G)$

Primal formulation:

$$\Pi_{\mathfrak{B}_n}(G) = \arg\min \left\{ \frac{1}{2}\|X - G\|_F^2 \ \mid \ \mathcal{B}X = b, \ X \in C \right\}$$

$\mathcal{B}(X) = [Xe; \ X^T e]$, $C := \{X \in \Re^{n\times n} \mid X \geq 0\}$, $b = [e; e]$

Dual problem, convex differentiable function φ:

$$\min \left\{ \varphi(y) := \frac{1}{2}\|\Pi_C(\mathcal{B}^* y + G)\|_F^2 - \langle b, \, y\rangle - \frac{1}{2}\|G\|_F^2 \ \mid \ y \in \mathrm{Range}(\mathcal{B}) \right\}$$

$\Pi_{\mathfrak{B}_n}(G) = \Pi_C(\mathcal{B}^* \bar{y} + G)$ with $\bar{y} \in \arg\min_{y\in \mathrm{Range}(\mathcal{B})} \varphi(y)$

Simple convex QP, state-of-the-art commercial solvers (e.g., Gurobi, Mosek)

(accelerated) gradient methods, semismooth Newton methods

Newton's method

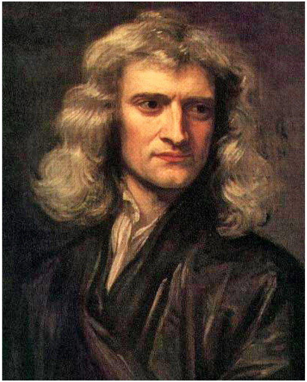


Figure: Sir Isaac Newton (Niu Dun) (4 January 1643 - 31 March 1727)

Which Newton's method?

Figure: Snail (Niu)

Figure: Longhorn beetle (Niu)

Figure: Charging Bull (Niu)

Figure: Yak (Niu)

Algorithm SSNCG

Recall $\nabla\varphi(y) = \mathcal{B}\Pi_C(\mathcal{B}^*y + G) - b, \quad \forall\, y \in \mathrm{Range}(\mathcal{B})$

SSNCG for nonsmooth equation:

$$\nabla\varphi(y) = 0, \quad y \in \mathrm{Range}(\mathcal{B})$$

j-th iter. Choose $\mathcal{V}_j \in \mathcal{B}\partial\Pi_C(\mathcal{B}^*y_j + G)\mathcal{B}^*$, solve linear system (CG)

$$(\mathcal{V}_j + \varepsilon_j I)d + \nabla\varphi(y^j) = 0, \quad d \in \mathrm{Range}(\mathcal{B})$$

$\varepsilon_j > 0$: small perturbation converging to zero.

Global convergence: Line search (using $\varphi(y)$)

Local convergence: at least superlinear if

$$\mathcal{B}\,\mathrm{lin}(\mathcal{T}_C(\Pi_C(\mathcal{B}^*\bar{y} + G)) = \mathrm{Range}(\mathcal{B})$$

SSNCG fast and robust

Numerical comparisons

Relative KKT residual: $\eta = \max\{\eta_P, \eta_C\}$,

$$\eta_P = \frac{\|\mathcal{B}X - b\|}{1 + \|b\|}, \quad \eta_C = \frac{\|X - \Pi_C(\mathcal{B}^* y + G)\|}{1 + \|X\|}$$

Algorithms: our semismooth Newton CG method (Ssncg), accelerated gradient, Gurobi

Test instances G:

1. `G = randn(n)`
2. Similarity matrices derived from LIBSVM datasets: **gisette**, **mushrooms**, **a6a**, **a7a**, **rcv1** and **a8a**

   normalize (unit l_2-norm), Gaussian kernel

$$G_{ij} = \exp\left(-\|x_i - x_j\|^2\right), \quad \forall\, 1 \le i, j \le n$$

Gurobi: default parameters

Ssncg and APG: terminate $\eta < \mathrm{tol}$ or the time exceeding 3 hours

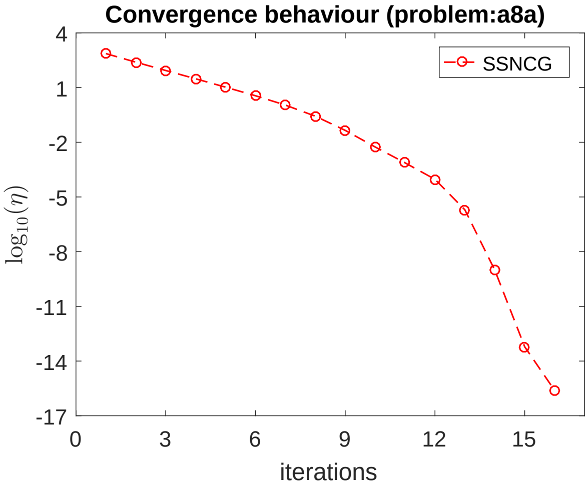
Numerical results

"a": Accelerated gradient ($\mathrm{tol} = 10^{-9}$), "b": Gurobi,

"c": SSNCG ($\mathrm{tol} = 10^{-15}$)

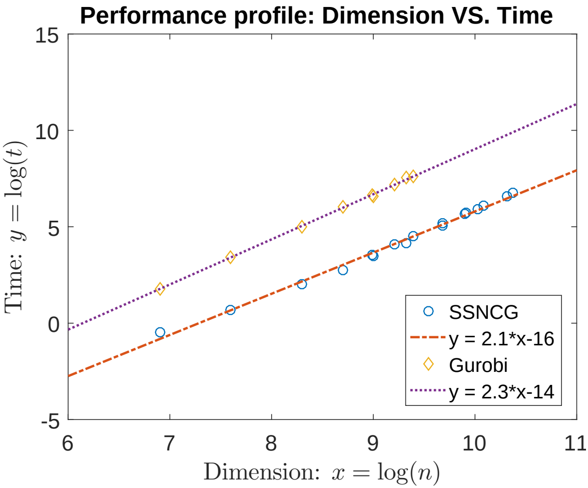
"*": Gurobi out of memory (128 G RAM)

		η	time
problem	n	a | b(η_P) | c	a | b | c
rand5	10000	**3.1-7** | **6.2-6** (3.4-15) | 4.5-16	3:00:00 | 21:27 | 58
rand6	12000	**2.6-4** | **4.6-6** (3.8-15) | 4.6-16	3:00:00 | 33:31 | 1:33
rand9	24000	**1.9-2** | * | 4.9-16	3:00:04 | * | 7:15
rand10	30000	**4.9-2** | * | 5.9-16	3:00:14 | * | 12:01
rand11	32000	**6.3-2** | * | 4.8-16	3:00:17 | * | 14:10
gisette	6000	9.8-10 | **3.3-6** (2.5-15) | 6.5-16	7:19 | 6:58 | 16
mushrooms	8124	9.8-10 | **9.5-5** (4.8-15) | 1.9-16	11:07 | 11:58 | 32
a6a	11220	9.9-10 | **4.7-6** (4.0-15) | 3.8-16	34:29 | 31:21 | 1:03
a7a	16100	9.9-10 | * | 2.9-16	1:28:14 | * | 2:34
rcv1	20242	**1.3-6** | * | 1.9-16	3:00:03 | * | 5:02
a8a	22696	**2.7-4** | * | 2.5-16	3:00:03 | * | 6:15



Superlinear convergence of SSNCG

Performance profile



Computational complexities:

$$t_{\text{Ssncg}} = \mathcal{O}(n^{2.1}), \quad t_{\text{Gurobi}} = \mathcal{O}(n^{2.3}), \quad \frac{t_{\text{Gurobi}}}{t_{\text{Ssncg}}} = 7n^{0.2}$$

SsnCG VS. PPROJ

PPROJ: C codes, extremely fast implementation, algorithm for projection onto general polyhedral sets [Hager & Zhang, SIOPT, 2016]

"a": PPROJ, "b": SsnCG ($\mathrm{tol} = 10^{-15}$)

Executed on HPC clusters in NUS

		η	time
problem	n	a | b	a | b
rand5	10000	5.8-12 | 4.5-16	3:45 | 39
rand6	12000	1.6-12 | 4.7-16	5:31 | 59
rand7	16000	5.8-13 | 5.9-16	19:34 | 1:20
rand8	20000	4.3-13 | 9.5-16	34:01 | 2:10
gisette	6000	1.4-14 | 6.5-16	2:39 | 11
mushrooms	8124	**6.9-7** | 2.0-16	16:22:46 | 21
a6a	11220	3.3-14 | 3.8-16	14:32 | 39
a7a	16100	3.7-14 | 2.9-16	43:53 | 1:21
rcv1	20242	1.3-13 | 1.9-16	2:01:32 | 2:19

Generalized Jacobian of $\Pi_D(\cdot)$

$\partial \Pi_{\mathfrak{B}_n}(G)$: second order algorithms for optimization over $\mathfrak{B}_n$

Polyhedral $D := \{x \in \Re^n \mid Ax \geq b,\ Bx = d\}$, B full row rank

For any $x \in \Re^n$, KKT condition for $\Pi_D(x)$

$$\begin{cases} \Pi_D(x) - x + A^T\lambda + B^T\mu = 0, \\ A\Pi_D(x) - b \geq 0, \quad B\Pi_D(x) - d = 0, \\ \lambda \leq 0, \quad \lambda^T(A\Pi_D(x) - b) = 0 \end{cases} \tag{1}$$

Multipliers $M(x) := \{(\lambda, \mu) \in \Re^m \times \Re^p \mid (x, \lambda, \mu) \text{ satisfies } (1)\}$

Active index $I(x) := \{i \mid A_i\Pi_D(x) = b_i,\ i = 1, \ldots, m\}$

$\Pi_D(\cdot)$: non-smooth, piecewise-affine, difficult to find elements in $\partial \Pi_D(x)$

Any computable approach?

Generalized Jacobian of $\Pi_D(\cdot)$

A_K: rows of A, indexed by K

$$\mathcal{D}(x) := \{\ K \subseteq [1:m] \mid \exists\, (\lambda,\mu) \in M(x) \text{ s.t. } \operatorname{supp}(\lambda) \subseteq K \subseteq I(x), \\ [A_K^T\ \ B^T] \text{ is of full column rank}\}$$

$$\mathcal{P}(x) := \left\{ \begin{array}{l} P \in \Re^{n\times n} \mid \\ P = I_n - [A_K^T\ \ B^T]\left(\begin{bmatrix} A_K \\ B \end{bmatrix} [A_K^T\ \ B^T]\right)^{-1} \begin{bmatrix} A_K \\ B \end{bmatrix},\ K \in \mathcal{D}(x) \end{array} \right\}$$

$\mathcal{P}(\cdot)$: Upper semicontinuity, [Han & Sun, JOTA, 1997]

Semismooth Newton method: find an element in $\mathcal{P}(x)$

Difficulties:

1. K corresponds to λ, λ unavailable
2. full column rank of $[A_K^T\ \ B^T]$

HS-Jacobian of Π_D

Theorem 1

For any given $x \in \Re^n$, denote

$$P_{HS} := I_n - [A_{I(x)}^T \;\; B^T] \left(\begin{bmatrix} A_{I(x)} \\ B \end{bmatrix} [A_{I(x)}^T \;\; B^T] \right)^{\dagger} \begin{bmatrix} A_{I(x)} \\ B \end{bmatrix}.$$

Then, $P_{HS} \in \mathcal{P}(x)$.

P_{HS}: referred to as HS-Jacobian (HS: Han & Sun)

Advantages of P_{HS}:

1. unrelated to index sets K and multipliers λ
2. full column rank assumption removed

HS-Jacobian of $\Pi_{\mathfrak{B}_n}$

Given $G \in \Re^{n\times n}$, denote $\overline{G} := \Pi_{\mathfrak{B}_n}(G)$

Linear operator $\Xi : \Re^{n\times n} \to \Re^{n\times n}$

$$\Xi(H) := \Theta \circ H, \quad H \in \Re^{n\times n}, \quad \Theta_{ij} = \begin{cases} 0, & \text{if } \overline{G}_{ij} = 0, \\ 1, & \text{otherwise.} \end{cases}$$

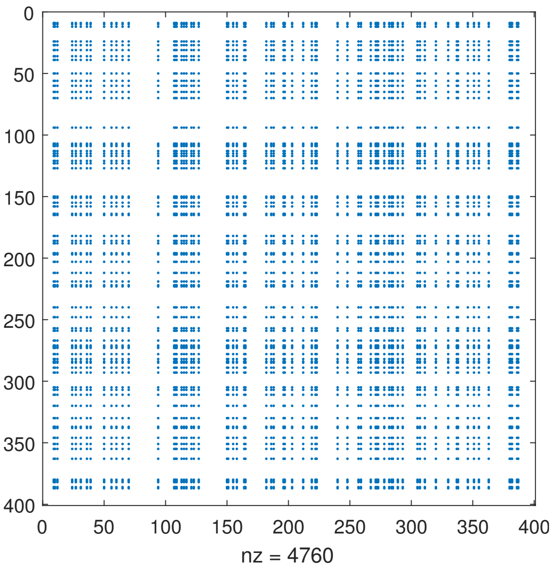
Proposition 1

The linear operator $P_{HS} : \Re^{n\times n} \to \Re^{n\times n}$ given by

$$P_{HS}(H) := \Xi(H) - \Xi\mathcal{B}^*(\mathcal{B}\Xi\mathcal{B}^*)^\dagger \mathcal{B}\Xi(H), \quad \forall\, H \in \Re^{n\times n},$$

is the HS-Jocobian of $\Pi_{\mathfrak{B}_n}$ at G.

Sparsity of HS-Jacobian of $\Pi_{\mathfrak{B}_n}$



$$n = 20, \quad P_{HS} \in \Re^{n^2 \times n^2}, \quad \text{sparsity} = 0.0297$$

QP with Birkhoff polytope constraints

Convex QP:

$$(\mathbf{P}) \quad \min \left\{ \frac{1}{2}\langle X,\, \mathcal{Q}X\rangle + \langle G,\, X\rangle \mid X \in \mathfrak{B}_n \right\},$$

Self-adjoint linear operator $\mathcal{Q} \succeq 0$

$$(\mathbf{D}) \min \left\{ \delta^*_{\mathfrak{B}_n}(Z) + \frac{1}{2}\langle W,\, \mathcal{Q}W\rangle \mid Z + \mathcal{Q}W + G = 0,\, W \in \mathrm{Range}(\mathcal{Q}) \right\}$$

$\delta^*_{\mathfrak{B}_n}$: the conjugate of the indicator function $\delta_{\mathfrak{B}_n}$

ALM function for **(D)**, given $\sigma > 0$

$$\mathcal{L}_\sigma(Z, W; X) = \delta^*_{\mathfrak{B}_n}(Z) + \frac{1}{2}\langle W,\, \mathcal{Q}W\rangle - \langle X,\, Z + \mathcal{Q}W + G\rangle + \frac{\sigma}{2}\|Z + \mathcal{Q}W + G\|^2$$

ALM for (D)

Algorithm ALM: An augmented Lagrangian method for (D).

Given $\sigma_0 > 0$, iterates $k = 0, 1, \ldots$

Step 1. Compute

$$(Z^{k+1}, W^{k+1}) \approx \operatorname{argmin} \left\{ \begin{array}{l} \Psi_k(Z, W) := \mathcal{L}_{\sigma_k}(Z, W; X^k) \\ \mid (Z, W) \in \Re^{n\times n} \times \text{Range}(\mathcal{Q}) \end{array} \right\}.$$

Step 2. Compute

$$X^{k+1} = X^k - \sigma_k(Z^{k+1} + \mathcal{Q}W^{k+1} + G).$$

Update $\sigma_{k+1} \uparrow \sigma_\infty \leq \infty$.

Convex piecewise linear-quadratic minimization:

error bound holds $\Longrightarrow$ ALM converges asymptotically superlinearly

Semismooth Newton method CG for inner problem

For any $W \in \mathrm{Range}(\mathcal{Q})$,

$$\psi(W) := \inf_{Z} \mathcal{L}_\sigma(Z, W; \widehat{X}), \quad Z(W) := \widehat{X} - \sigma(\mathcal{Q}W + G)$$

Subproblem solution $(\overline{Z}, \overline{W})$:

$$\overline{W} = \arg\min \left\{ \psi(W) \ | \ W \in \mathrm{Range}(\mathcal{Q}) \right\},$$
$$\overline{Z} = \sigma^{-1}\big(Z(\overline{W}) - \Pi_{\mathfrak{B}_n}(Z(\overline{W}))\big)$$

For all $W \in \mathrm{Range}(\mathcal{Q})$,

$$\nabla\psi(W) = \mathcal{Q}W - \mathcal{Q}\Pi_{\mathfrak{B}_n}(Z(W))$$

Semismooth Newton CG solve nonsmooth piecewise affine equation

$$\nabla\psi(W) = 0, \quad W \in \mathrm{Range}(\mathcal{Q}).$$

Semismooth Newton method CG for inner problem

Given $\widehat{W}$, linear operator $\mathcal{M} : \Re^{n\times n} \to \Re^{n\times n}$

$$\mathcal{M}(\Delta W) := (\mathcal{Q} + \sigma \mathcal{Q} P_{HS} \mathcal{Q})\Delta W, \quad \forall \Delta W \in \Re^{n\times n}$$

P_{HS}: the HS-Jacobian of $\Pi_{\mathfrak{B}_n}$ at $Z(\widehat{W})$

j-th iter., solve linear system (CG)

$$\mathcal{M}_j dW + \nabla \psi(W^j) = 0, \quad dW \in \text{Range}(\mathcal{Q})$$

Global convergence: Line search (using $\psi(W)$)

Local convergence:
positive definiteness of $\mathcal{M}$ on $\text{Range}(\mathcal{Q})$ $\Longrightarrow$ at least superlinear

Numerical results

Given $A, B \in \mathcal{S}^n$, QAP:

$$\min\{\langle X,\ AXB\rangle \mid X \in \{0,1\}^{n\times n} \cap \mathfrak{B}_n\}$$

Convex relaxation [Anstreicher et al. MP, 2001]:

$$\min\{\langle X,\ \mathcal{Q}X\rangle \mid X \in \mathfrak{B}_n\}$$

Self-adjoint linear operator $\mathcal{Q}(X) := AXB - SX - XT, \quad \mathcal{Q} \succeq 0$

Matrices $S, T \in \mathcal{S}^n$ obtained from [Anstreicher et al. MP, 2001]

Relative KKT residual:

$$\eta = \frac{\|X - \Pi_{\mathfrak{B}_n}(X - \mathcal{Q}X)\|}{1 + \|X\| + \|\mathcal{Q}X\|}$$

Matrices A, B from QAPLIB

Numerical results for QAP

"a": Gurobi, "b": ALM

		iter	η	time
problem	n	a | b (itersub)	a|b	a|b
lipa80a	80	11 | 25 (68)	1.3-6 | 7.3-8	2:46 | 01
lipa90a	90	11 | 20 (54)	2.7-6 | 8.8-8	5:32 | 01
sko100a	100	14 | 26 (95)	8.5-6 | 8.5-8	2:06 | 11
tai100a	100	11 | 18 (52)	1.3-6 | 9.5-8	10:31 | 02
tai100b	100	11 | 27 (98)	1.3-6 | 9.1-8	10:31 | 13
tai80b	80	11 | 27 (98)	1.2-6 | 8.5-8	2:36 | 07
tai256c	256	* | 2 (4)	* | 2.1-16	* | 00
tai150b	150	19 | 27 (94)	4.3-7 | 9.3-8	2:46:17 | 13
tho150	150	16 | 24 (96)	5.6-6 | 9.9-8	18:52 | 22

"*": Gurobi out of memory (128 G RAM)

"tai150b": Gurobi reports error, "small positive term" needed

References

[Defeng Sun, Houdou Qi], A quadratically convergent Newton method for computing the nearest correlation matrix, SIMAX, 2006

[Xudong Li, Defeng Sun, Kim-Chuan Toh], On the efficient computation of a generalized Jacobian of the projector over the Birkhoff polytope, arXiv:1702.05934, 2017

Thank you for your attention!